Abstract Submitted
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Full-dimensional, permutationally invariant and size-extensive potential energy surfaces for small molecules[1] B.J. BRAAMS, Dept. of Math. and CS, Emory Univ., JOEL M. BOWMAN, ZHONG JIN, XINCHUAN HUANG, ZHEN XIE, PENG ZHANG, Dept. of Chemistry, Emory Univ., SEUNG PARK, Sungkyunkwan Univ., JOHN F. STANTON, MYCHEL VARNER, UT Austin — We have constructed full-dimensional potential energy surfaces for a variety of molecular systems, among them CH5+, H3O2-, H4O2, H5O2+, C2H2O, C3H3O, CH2O, and HOONO/HONO2. The property of invariance under permutations of like nuclei is built into the basis for the least-squares fitting procedure, and we relied on the MAGMA computational algebra system to find the invariants and to help generate the codes. The use of a cluster expansion (many-body expansion), going up to five-body or at most six-body terms, caters for dissociation and reaction processes and also for extension to larger systems. The fitted potential and its gradient are evaluated on a millisecond timescale, making it possible to do molecular dynamics or quantum Monte Carlo calculations at ab initio accuracy without anywhere near the cost that is normally associated with ab initio MD, or even with a Car-Parrinello treatment. We also use the fitted surface for MULTIMODE calculations of vibrational spectrum. The poster will present the computational approach and results for the mentioned systems.

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Bastiaan J. Braams
Emory University, Dept. of Math. and CS

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